GEO-SEQ Project
Quarterly Status and Cost Report
March 1 – May 31, 2003

Project Overview

The purpose of the GEO-SEQ Project is to establish a public-private R&D partnership that will:

- Lower the cost of geologic sequestration by: (1) developing innovative optimization methods for sequestration technologies with collateral economic benefits, such as enhanced oil recovery (EOR), enhanced gas recovery (EGR), and enhanced coalbed methane production; and (2) understanding and optimizing trade-offs between CO_2 separation and capture costs, compression and transportation costs, and geologic sequestration alternatives.
- Lower the risk of geologic sequestration by: (1) providing the information needed to select sites for safe and effective sequestration; (2) increasing confidence in the effectiveness and safety of sequestration by identifying and demonstrating cost-effective monitoring technologies; and (3) improving performance-assessment methods to predict and verify that long-term sequestration practices are safe, effective, and do not introduce any unintended environmental impact.
- Decrease the time to implementation by: (1) pursuing early opportunities for pilot tests with our private-sector partners and (2) gaining public acceptance.

In May 2000, a project kickoff meeting was held at Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab) to plan the technical work to be carried out, starting with FY00 funding allocations. Since then, work has been performed on four tasks: (A) development of sequestration co-optimization methods for EOR, depleted gas reservoirs, and brine formations; (B) evaluation and demonstration of monitoring technologies for verification, optimization, and safety; (C) enhancement and comparison of computer-simulation models for predicting, assessing, and optimizing geologic sequestration in brine, oil, and gas, as well as coalbed methane formations; and (D) improvement of the methodology and information available for capacity assessment of sequestration sites. Recently, a new task in support of the Frio Brine Pilot Project (E) has been added.

This Quarter's Highlights

- Members of the technical and scientific team for the Frio Brine Pilot Project (Task E) met on April 23–24 in Houston, Texas, to develop more detailed plans for integrating the different GEO-SEQ Project task experiments with the well design and test schedule.
- The first reactive transport experiment intended to validate Lawrence Livermore National Laboratory's (LLNL's) reactive transport simulators and to aid in the design of the Frio Brine Pilot Project (Task E) was completed.
- A remotely controlled electrical-resistance tomography (ERT) data acquisition system was successfully tested and deployed in the field. The capability of obtaining full time-lapse datasets on command, will allow completion of frequent surveys to monitor changes in the field resulting from CO_2 injection.
- Numerical simulation studies of co-optimization of oil recovery and CO_2 storage showed that one problem with gas injection is the high mobility of the CO_2 as compared to the native/*in situ* reservoir fluids. This problem leads to premature breakthrough of CO_2 at the production wells and an incomplete reservoir sweep. These effects may be reduced by appropriate operation of the production wells (see Subtask A-1).
- Data analysis of the Lost Hills, California, CO_2 injection test indicate that the contribution of injectate CO_2 to the system can be quantified; the changes correlate with periods of CO_2 injection and water flooding.
- Comparisons continued of results of different simulation problems related to CO_2 sequestration in deep, unmineable coal seams.

- At the National Energy Technology Laboratory (NETL) Second National Conference on Carbon Sequestration (May 5–8, Alexandria, Virginia), nine papers were presented describing different studies being performed as part of the GEO-SEQ Project.
- Grid effects (i.e., grid orientation, uniformity, and resolution) on the results of numerical simulation of CO_2 injection and storage were analyzed. The study showed that spurious preferential flow in the grid axis directions is increased by the coarsening of the grid away from the wells. This effect further distorts the shape of the injectate plume resulting from numerical dispersion.

Papers Presented, Submitted, Accepted, or Published during This Quarter

Cole, D.R., J. Horita, M.C. van Soest, B.M. Kennedy, and M.F. Morea, Gas chemistry and isotope monitoring during the Lost Hills, California, CO_2 injection test. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003.

Doughty, C., and K. Pruess. Modeling supercritical CO_2 injection in heterogeneous porous media. Paper Presented at the TOUGH Symposium 2003, Berkeley, California, May 12–14, 2003; Berkeley Lab Report LBNL-52527, 2003.

Doughty, C., S.M. Benson, and K. Pruess, Development of a well-testing program for a CO_2 sequestration pilot in a brine formation. Paper Presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003.

Fisher, L.S., D.R. Cole, J.G. Blencoe, G.R. Moline, J.C. Parker, and T.J. Phelps, High-pressure flow-through column for assessing subsurface carbon sequestration. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003.

Hoversten, G., M., R. Gritto, J. Washbourne, and T.M. Daley, Pressure and fluid saturation prediction in a multicomponent reservoir, using combined seismic and electromagnetic imaging. *Geophysics* (in press); Berkeley Lab Report LNBL-51281, 2003.

Hovorka, S. D., C. Doughty, S.M. Benson, S. M., K. Pruess, and P.R. Knox. Assessment of the impact of geological heterogeneity on CO2 storage in brine formations: a case study from the Texas Gulf Coast. In Geological storage for Emissions Reduction: Technology (S.J. Baines, J.Gale and R.H. Worden, eds), Geological Society (London) Special publication (in press), 2003.

Hovorka, S.D., P.R. Knox, M.H. Holtz, J.S.Yeh, K. Fouad, and S. Sakurai, Tapping the potential for large volume sequestration—Update on the Frio Brine Pilot Project. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003.

Hovorka, S.D., P.R. Knox, and J.A. Raney. What does a permit look like for disposal of carbon dioxide waste plus enhanced recovery of oil and gas? Paper and talk presented to UIC Conventions at TCEQ Trade Show, Austin, Texas, May 5, 2003.

Holtz, M.H., Optimization of CO_2 sequestered as a residual phase in brine-saturated formations. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003.

Holtz, M.H., Pore-scale influences on saline aquifer CO_2 sequestration. Paper presented at the AAPG Annual Meeting 2003, Salt Lake City, Utah, May 11–14, 2003.

Johnson, J.W., J.J. Nitao, R.L. Newmark, B.A. Kirkendall, G.J. Nimz, and K.G. Knauss. Geologic approaches to carbon management: CO_2-flood EOR and saline aquifer storage. Paper presented at the 28th International Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, March 10–13, 2003.

Johnson, J.W., J.J. Nitao, and J.P. Morris. Reactive transport modeling of long-term cap rock integrity during CO_2 injection for EOR or saline-aquifer storage. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003.

Knauss, K.G., J.W. Johnson and C.I. Steefel. Evaluation of the impact of CO_2, co-contaminant aqueous fluid, and reservoir rock interactions on the geologic sequestration of CO_2. Paper presented at the 28th International Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, March 10–13, 2003.

Knauss, K.G., J.W. Johnson, and C.I. Steefel. CO_2 sequestration in the Frio FM TX: Evaluation of the impact of CO_2, co-contaminant gas, aqueous fluid, and reservoir rock interactions. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003,.

Knox, P.R., C. Doughty, and S.D. Hovorka. Impacts of buoyancy and pressure gradient on field-scale geological sequestration of CO_2 in saline formations. Paper presented at AAPG Annual Meeting 2003, Salt Lake City, Utah, May 11–14, 2003; Berkeley Lab Report LBNL-51510 (abstract), 2003.

Law, D.H-S, GEO-SEQ project, numerical model comparison study for greenhouse sequestration in coalbeds—An update. Paper presented at the Coal-Seq II Forum, Washington, D.C., March 6–7, 2003.

Law, D.H.-S., L.G.H. (Bert) van der Meer and W.D.(Bill) Gunter, Comparison simulators for greenhouse gas sequestration in coalbeds, Part III: More complex problems. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003.

Oldenburg, C.M., S.H. Stevens, and S.M. Benson, Economic feasibility of carbon sequestration with enhanced gas recovery (CSEGR). Energy, 2003 (in press); Berkeley Lab Report LBNL-49762, 2003.

Oldenburg, C.M., S.W. Webb, K. Pruess, and G.J. Moridis, Mixing of stably stratified gases in subsurface reservoirs: A comparison of diffusion models. Transport in Porous Media, 2003 (in press); Berkeley Lab Report LBNL-51545, 2003.

Pruess, K., J. García, T. Kovscek, C. Oldenburg, J. Rutqvist, C. Steefel, and T. Xu, Code intercomparison builds confidence in numerical simulation models for geologic disposal of CO_2. Energy, 2003 (in press); Berkeley Lab Report LBNL-52211, 2003.

Rau. G.H., K.G. Knauss, and K. Caldera, Capturing and sequestering flue-gas CO_2 using a wet limestone scrubber. Paper presented at NETL's Second National Conference on Carbon Sequestration, Alexandria, Virginia, May 5–8, 2003,

Zhu, J., K. Jessen, A. R. Kovscek, and F.M. Orr, Jr., Analytical theory of coalbed methane recovery by gas injection. Society of Petroleum Engineers Journal, 2003 (submitted).

Task Summaries

Task A: Develop Sequestration Co-Optimization Methods

Subtask A-1: Co-Optimization of Carbon Sequestration, EOR, and EGR from Oil Reservoirs

Goals

To assess the possibilities for co-optimization of CO_2 sequestration and enhanced oil recovery (EOR), and to develop techniques for selecting the optimum gas composition for injection. Results will lay the groundwork necessary for rapidly evaluating the performance of candidate sequestration sites, as well as monitoring the performance of CO_2 EOR.

Previous Main Achievements

- Screening criteria for selection of oil reservoirs that would co-optimize EOR and maximize CO_2 storage in a reservoir have been generated.
- A streamline-based proxy for full reservoir simulation has been thoroughly studied. It allows rapid selection of a representative subset of stochastically generated reservoir models that encompass uncertainty with respect to true reservoir geology.
- Reservoir simulation studies of co-optimization have shown that storage of CO_2 can be increased, with little or no loss in oil production, through active control of injection and production conditions while injecting pure CO_2.

Accomplishments This Quarter

Numerical simulation work studying co-optimization of oil recovery and CO_2 storage confirmed that a problem with gas injection is the high mobility of the CO_2 compared to the native/in situ reservoir fluids. The adverse mobility ratios result in premature breakthrough of CO_2 at the production wells and in an incomplete reservoir sweep. These effects may be reduced by shutting in and then opening the producers as they reach given gas-oil ratios and pressures (see below).

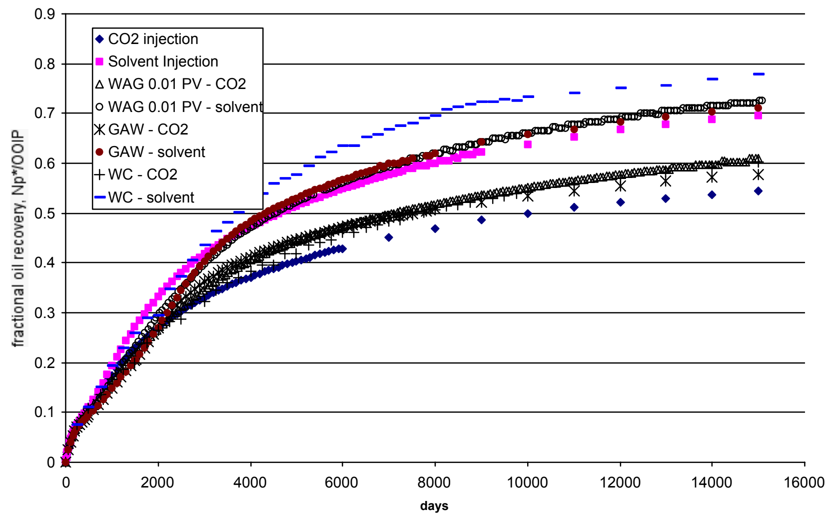
Progress This Quarter

Previously, we developed a synthetic three-dimensional model of an oil reservoir including a compositional reservoir fluid description. The reservoir model is a realistic three-dimensional, heterogeneous, and stochastic description that includes a 15-component reservoir fluid. Reservoir shape is anticlinal, with faults and an aquifer bounding it. The description of heterogeneities and their distribution is geostatistical in that multiple reservoir models are generated that capture variability and uncertainty. There are four injectors near the flanks of the reservoir and four producers near the crest. The reservoir does not represent a typical CO_2 injection candidate: the oil is relatively heavy (24°API), and pure CO_2 is not miscible in the crude oil at reservoir pressure. In some sense, our work expands the range of applicability for CO_2 injection.

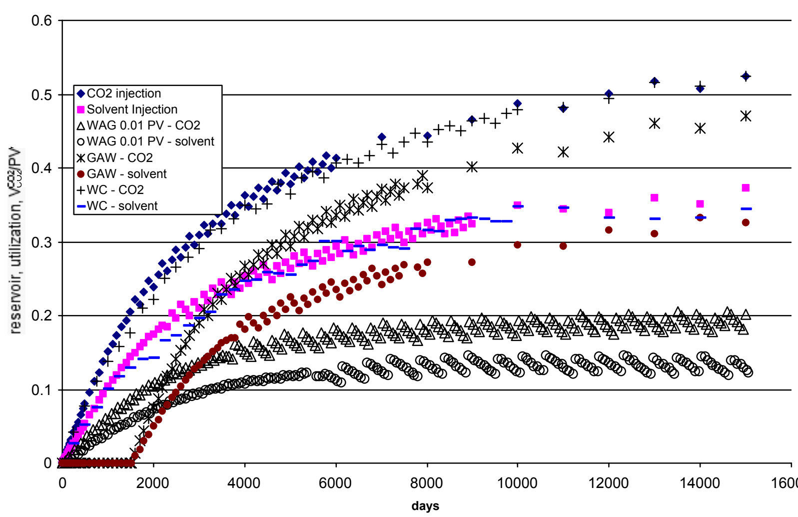
This synthetic reservoir has been subjected to various reservoir development scenarios (via reservoir simulation), allowing us to explore development and production techniques that would maximize simultaneous production of oil and CO_2 storage. Our co-optimization goals were focused partially on establishing that at least as much oil as in conventional recovery could be produced, and that co-optimization results were not specific to a particular reservoir model. Briefly, we are examining water-alternating-gas (WAG) drive mode, gas injection early in production life (versus late in reservoir life), gas injection following waterflooding (GAW), and gas-controlled production (WC).

The first two scenarios are designed so that the mobilities of the injected phases in the reservoir are reduced. In the last scenario, production wells are actively controlled to limit the amount of produced gas and increase the contact of gas with reservoir volume. Control parameters are the producing gas-oil ratio (GOR) and the injection pressure. In all cases, oil production is discounted by the equivalent amount of energy needed to compress produced gas. Schemes that incur excessive gas cycling pay a penalty with respect to oil production. We have used both pure CO_2 as an immiscible injection gas and a miscible solvent mixture that is 2/3 (by mole) CO_2.

Typical results are displayed in **Figure 1**. **Figure 1(a)** shows oil recovery versus time, whereas **Figure 1(b)** displays the fraction of the total reservoir volume filled with CO_2. As **Figure 1(a)** shows, oil recovery is greatest as a result of miscible gas injection. With miscible gas injection, the local displacement efficiency approaches unity, and recovery is maximized. Among the scenarios with miscible gas injection, well-controlled injection resulted in oil recovery 7 to 12% greater than the other cases and approaches 80% of the oil in place. In the case of pure CO_2 injection, WAG with small equal-sized slugs (0.01 pore volume) of water and CO_2 performs the best. Ultimate recovery, however, is virtually the same as well-controlled CO_2 injection. The main differences between these two scenarios are found during intermediate portions of the recovery, lying between 3,000 and 7,000 days.



(a)



(b)

Figure 1. (a) Oil recovery and (b) reservoir utilization of various gas-injection strategies. Oil recovery is discounted by the equivalent energy necessary to compress any produced injection gases. In **Figure 1(b)**, the injection scenarios are compared with respect to the reservoir volume utilized. In this case, immiscible CO2 injection cases perform better than miscible solvent injection because only two-thirds of the solvent gas by mole is CO2. All cases illustrate that injection of water for mobility control frustrates sequestration. Pore space becomes filled with water when it otherwise could be filled with CO2.

Gas-controlled production appears promising. Oil production obtained from pure CO_2 injection with well control is on a par with that obtained in an optimized WAG process, whereas the utilization of reservoir volume to store CO_2 is about 2.5 times that of a WAG scheme. Gas-controlled production appears to limit gas cycling while increasing oil production and CO_2 storage by 12 to 20% compared to injecting pure CO_2 or solvent gas. The well-controlled gas production scheme has been applied to a series of reservoir models and been found to give good results in all cases. In short, well-controlled gas production appears to meet the criteria for co-optimization: oil recovery similar to a conventional recovery process, good volumetric utilization of a reservoir, continuous injection of CO_2, and limited cycling of injectate.

Figure 1(a) also makes clear that a common problem with gas injection is the high mobility of the CO_2 as compared to the resident fluids (see the results for CO_2 injection). Adverse mobility ratios lead to premature breakthrough of CO_2 at production wells and incomplete sweep of reservoir volume. Aqueous foams have the ability to profoundly alter the mobility of injected gas. To this end, we have been conducting experiments to measure the trapping of CO_2 by foam. X-ray CT scanning monitors experimental progress.

We measure the fraction of gas that is stationary using a dual-gas tracer technique. Experimentally, gas and liquid injection rates are set for a given surfactant concentration and a measurement of the stationary gas saturation obtained at steady state. By adjusting injection conditions, we make a series of measurements. **Figure 2** summarizes some results obtained to date. Trapped gas fraction is plotted versus the steady-state pressure drop. Notice that the fraction of gas that is stationary can be in excess of 90%. At small pressure drops that are characteristic of regions far away from wells, most of the gas should be held stationary by the foam. Thus, gas mobility is greatly reduced, and reservoir utilization should increase.

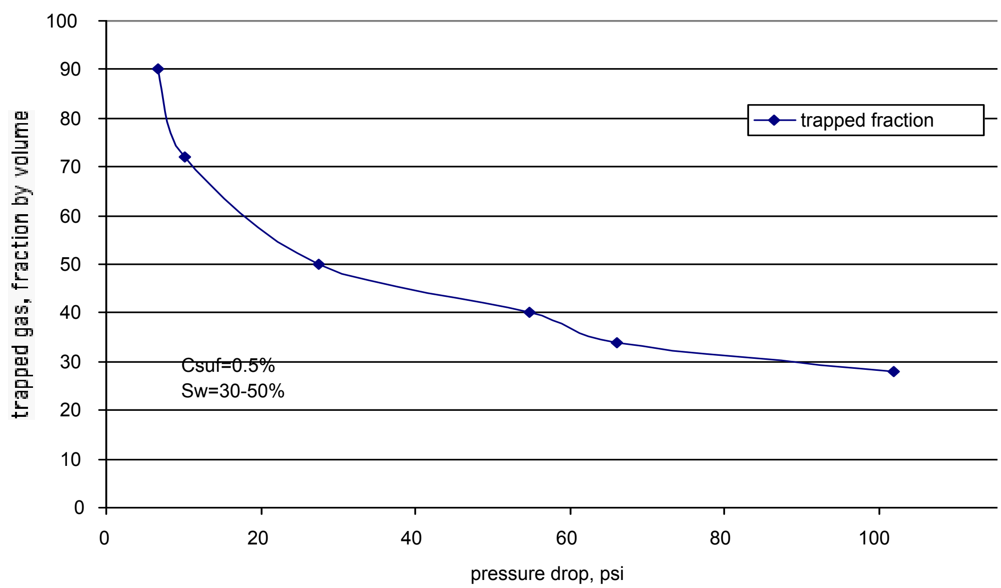


Figure 2. Trapped gas versus gas injection rate.

Work Next Quarter

Our co-optimization results, including the creation of the synthetic reservoir, will be written up for journal submission. Further work will consider the best set of control parameters for well-controlled gas injection. For instance, injection pressure and producing gas-oil ratio were used, but we can also consider other parameters such as the liquid saturation around production wells. We also intend to consider the optimal placement of wells to maximize simultaneous oil production and CO_2 storage.

The experimental effort on CO_2 trapping by foam will continue. We are in the midst of a series of experiments to characterize the mobile fraction of a foamed gas as a function of pressure drop, surfactant concentration, etc. The *in situ* distribution of CO_2 is imaged using x-ray computed tomography.

Subtask A-2: Feasibility Assessment of Carbon Sequestration with Enhanced Gas Recovery (CSEGR) in Depleted Gas Reservoirs

Goals

To assess the feasibility of injecting CO_2 into depleted natural gas reservoirs for sequestering carbon dioxide (CO_2) and enhancing methane (CH_4) recovery. Investigation will include assessments of (1) CO_2 and CH_4 flow and transport processes, (2) injection strategies that retard mixing, (3) novel approaches to inhibit mixing, and (4) identification of candidate sites for a pilot study.

Previous Main Achievements

On the basis of numerical-simulation studies, the proof-of-concept for CO_2 storage with enhanced gas recovery (CSEGR) was demonstrated and the economic feasibility of these projects was evaluated

It was found that transport in a high-permeability gas reservoir could be adequately simulated using the Advective Diffusive Model (ADM), but that the Dusty Gas Model (DGM) is more appropriate for lower permeability units.

Accomplishments This Quarter

Several contacts were made to identify potential CSEGR pilot sites in the U.S., and collaboration with European colleagues working on CSEGR continued.

Progress This Quarter

Earlier, we had identified a potential CSEGR site in Texas owned by Samson Resources, not far from the upcoming Frio CO_2 injection test. Unfortunately, the company's management objected to the idea, because (1) the site is mostly an oil field and (2) they were concerned about old metal pipe in the ground being corroded by the injected CO_2. Michael Milliken (Sampson Resources) suggested we look for a site around the city of Monroe, northeastern Louisiana, where there are several depleted and shut-in gas reservoirs.

Hugh Sharma of Denmark, who is working on CO_2 injection for EOR in the North Sea project (CENS), contacted us. He is interested in expanding the scope of their project to include enhanced gas recovery (EGR). We have just begun corresponding with him about CSEGR.

We have been helping a visiting scientist, Dr. Dorothee Rebscher; prepare to run simulations of CSEGR for the Salzwedel-Peckenson gas reservoir in eastern Germany. Dr. Rebscher has assembled nearly all of the needed data and is close to developing the reservoir model in preparation for CSEGR simulations.

Work Next Quarter

- Look into the possibility of developing a CSEGR pilot site at one of the depleted gas reservoirs near Monroe, Louisiana, as recommended by Samson Resources. With the assistance of other interested parties, continue the search of other potential sites.
- Test and verify the newly developed solubility model that will be incorporated into TOUGH2/EOS7C. The new model handles multicomponent gas mixtures and will be more accurate at high pressures (>50 bar) than the one we have at present.
- Verify enthalpy calculations in TOUGH2/EOS&C and design a research plan to investigate non-isothermal effects on CO_2 injection.

Subtask A-3: Evaluation of the Impact of CO2 Aqueous Fluid and Reservoir Rock Interactions on the Geologic Sequestration of CO2, with Special Emphasis on Economic Implications.

Goals

To evaluate the impact on geologic sequestration of injecting an impure CO_2 waste stream into the storage formation. By reducing the costs of front-end processes, the overall costs of sequestration could be dramatically lowered. One approach is to sequester impure CO_2 waste streams that are less expensive or require less energy than separating pure CO_2 from the flue gas.

Previous Main Achievements

- Potential reaction products have been determined, based upon reaction-progress chemical thermodynamic/kinetic calculations for typical sandstone and carbonate reservoirs into which an impure CO_2 waste stream is injected.
- Reactive transport simulations have been completed for a plug-flow reactor (PFR) run using the Frio Formation core material acquired in support of Task E. Additional simulations were performed as part of the Frio Brine Pilot Project planning efforts (Task E).
- The PFR was upgraded by installing new pump-operating software.

Accomplishments This Quarter

- Completed the first reactive transport experiment intended to validate our reactive transport simulators and to aid in the design of the Frio Brine Pilot Project (Task E). This 30-day run in our upgraded PFR was intended to test the reactive transport simulator's capability to accurately model silicate mineral (clay) precipitation that could occur as a consequence of the injection of CO_2, an acid gas.

Progress This Quarter

We continued to evaluate the impact of waste stream CO_2, as well as contaminants (e.g., SO_2, NO_2, and H_2S), on injectivity and sequestration performance.

We also continued re-orienting our work to more directly support planning and execution of the Frio Pilot Project, being run in conjunction with the TBEG. To this end, at the April planning meeting held in Houston, we discussed geochemical sampling needs and potential sampling and analytical protocols with the ORNL geochemists, with whom we will be sharing responsibilities for field geochemical sample acquisition and analysis. We also discussed the possible use of space at the TBEG Houston Core Storage facility that could be used as lab space for analytical equipment. Analyses will be coordinated with the ORNL geochemists. Finally, we discussed possible laboratory pre-pilot tests with TBEG and SandiaTech personnel to evaluate the impact of CO_2 on grouts and cements in the injection well. This is required to ensure well seal integrity during the injection of CO_2, given that it produces quite low pH, aggressive solutions.

Unfortunately, we must rely on geochemical models (reactive transport simulators) to predict the long-term performance of CO_2 sequestration with respect to caprock seal integrity, given the relatively low kinetic rates of geochemical reactions at reservoir conditions. We cannot rely on the Frio Pilot project field experiment or laboratory experiments alone to assess performance. Validating our reactive transport simulators is a critical requirement, because of the long period over which containment must be assured. Our prior experience benchmarking reactive transport simulators against ideal reactive transport experiments (e.g., Johnson et al., 1998) suggests that our simulators handle dissolution of the more common rock-forming minerals reasonably well. However, these simulators have not been rigorously evaluated in terms of accurately modeling mineral growth. This is a serious shortcoming that we intend to address.

In the first of a planned series of PFR experiments specifically designed to address this problem, we have used a simulator (CRUNCH) to design an experiment that should produce a measurable amount of a clay mineral (kaolinite) reaction product under conditions directly relevant to CO_2 geologic sequestration. This issue is of some practical importance, because in the acidic conditions near the CO_2 injection well, the dissolution of silicate minerals could result in the growth of clay minerals that could decrease injectivity.

In both the experiment and the simulation, we used the composition of a Frio sand sample taken from well Merisol WDW No. 319. The starting mineralogy in the simulation consisted of a mix of quartz, K-feldspar, plagioclase (compositionally An60 with thermodynamic properties calculated as an ideal mixture of end members albite and anorthite), pyrite, muscovite (as a proxy for illite), kaolinite, clinochlore (as the Mg end-member chlorite), and calcite as the cement mineral. As a proxy for the formation fluid, we used a 0.7m NaCl solution, approximately equivalent to seawater in ionic strength. In the simulation and in the experiment this fluid was first equilibrated with 20b CO_2 gas pressure in an external Ti bomb (see Dec. 02–Feb. 03 GEOSEQ report for schematic) heated to run temperature (150°C—as explained below) that served to prime the precision Quizix pump. This priming further increased the fluid pressure to 80b before flowing it through the core contained in the tube furnace inside the PFR apparatus. In the experiment, quantitative samples of the effluent gas and liquid were collected frequently in gas tight syringes and analyzed for Ca, Mg, Na, K, Cl, Fe, CO_2, Al, Si and pH. In the simulation, of course, we can calculate not only the composition of the effluent exiting the core (i.e., the samples collected), but also the compositions of fluids, gases, and solids throughout the core in both space and time.

Because we use an ideal physical model (the PFR), we can set the simulation up as a very simple one-dimensional calculation. Because the incoming fluid is acidic due to the high CO_2 pressure (pH 3.7), we use full kinetic rate laws for each mineral, accounting for acid catalysis. Preliminary equilibrium modeling required speciating the model water at run initialization, suggested that possible secondary minerals included chalcedony, dawsonite, magnesite, and siderite. Under appropriate conditions, these minerals could precipitate, as well as any of the primary minerals, and kinetic rate laws also governed precipitation.

Our goal was to maximize the likelihood of producing quantifiable amounts of the expected secondary mineral kaolinite. Using the simulator as a test bed, we determined that by using a flow rate of 100 g/d for 30 days at a temperature of 150°C, we should produce enough new kaolinite distributed throughout the core so as to be easily quantified at the end of the simulated experiment. These conditions should also produce easily measurable compositional signals in the effluent, if our simulation is accurate. The reason for using a higher temperature than expected in a CO_2 sequestration reservoir is to try to accommodate any kinetic inhibition to mineral growth owing to nucleation effects, etc. We can do the experiment under “accelerated” conditions to make things happen conveniently fast. Our goal is to not only match the chemistry of the effluent through time, but also to match the distribution and composition of minerals throughout space at the end of the experiment.

As an example of the results of our *a priori* simulations and our reactive transport experiment, we show in **Figure 3** the calculated composition of the effluent as a function of time, as well as the actual measured solution composition determined in the acquired effluent samples from this experiment. The most important and obvious difference between simulation and observation is that predicted silica concentration is much lower than observed. The reason for the discrepancy is most likely that kaolinite growth has not, in fact, occurred, in spite of the simulation prediction. Instead, under these conditions we are only observing dissolution of the primary phases and no significant growth of any secondary minerals. This argument is strengthened by making a new simulation in which the growth of all secondary silica minerals is suppressed. **In Figure 4,** we plot the new calculated composition of the effluent as a function of time and (again) the actual measured solution composition determined in the acquired effluent samples. In this case, the correspondence between simulation and observation is much closer, suggesting that little, if any, kaolinite growth occurred during the experiment.

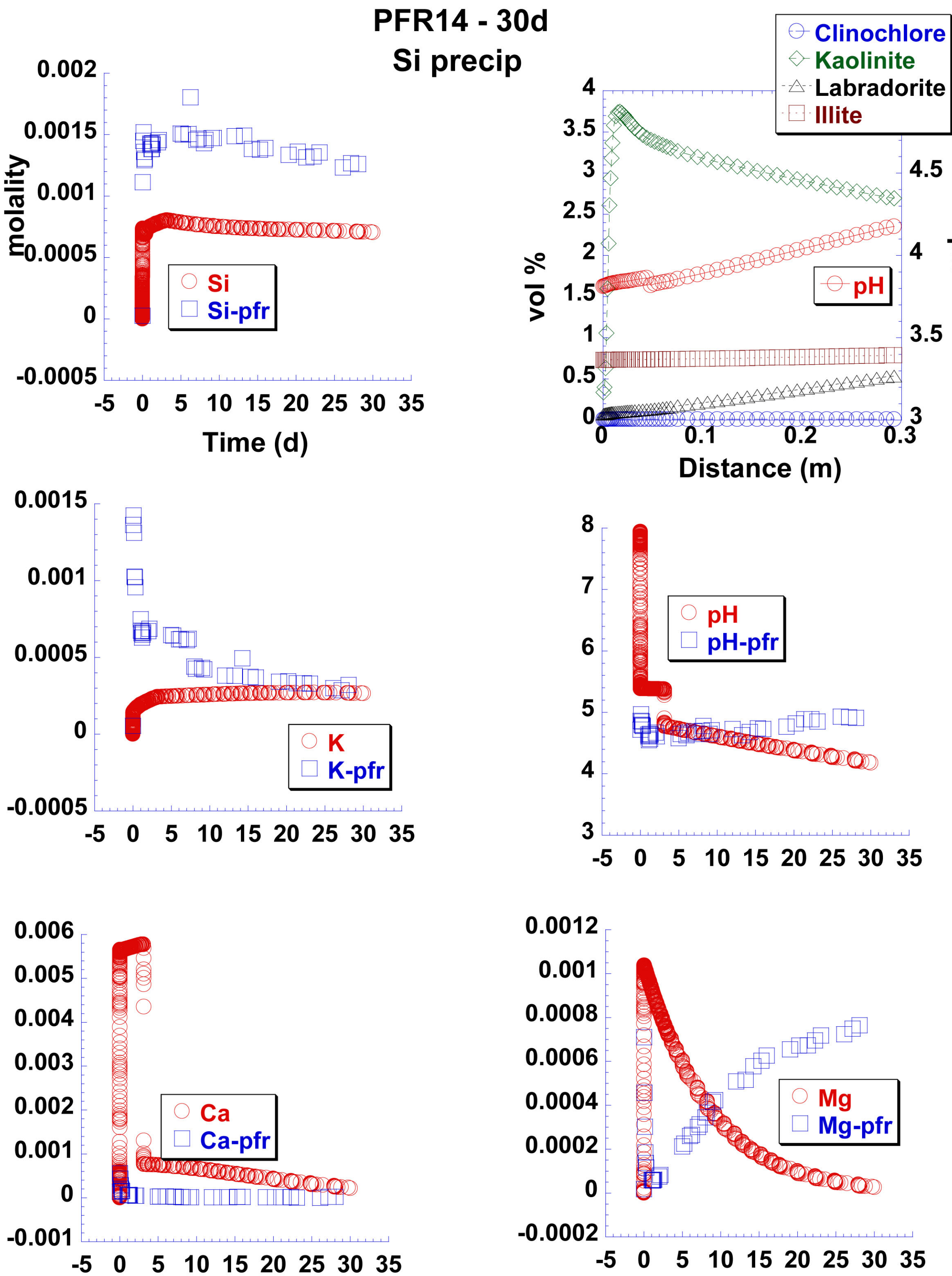


Figure 3. Reactive transport studies. All minerals are allowed to grow. With the exception of the upper right graph, simulated results are shown as squares and experimental ones as circles.

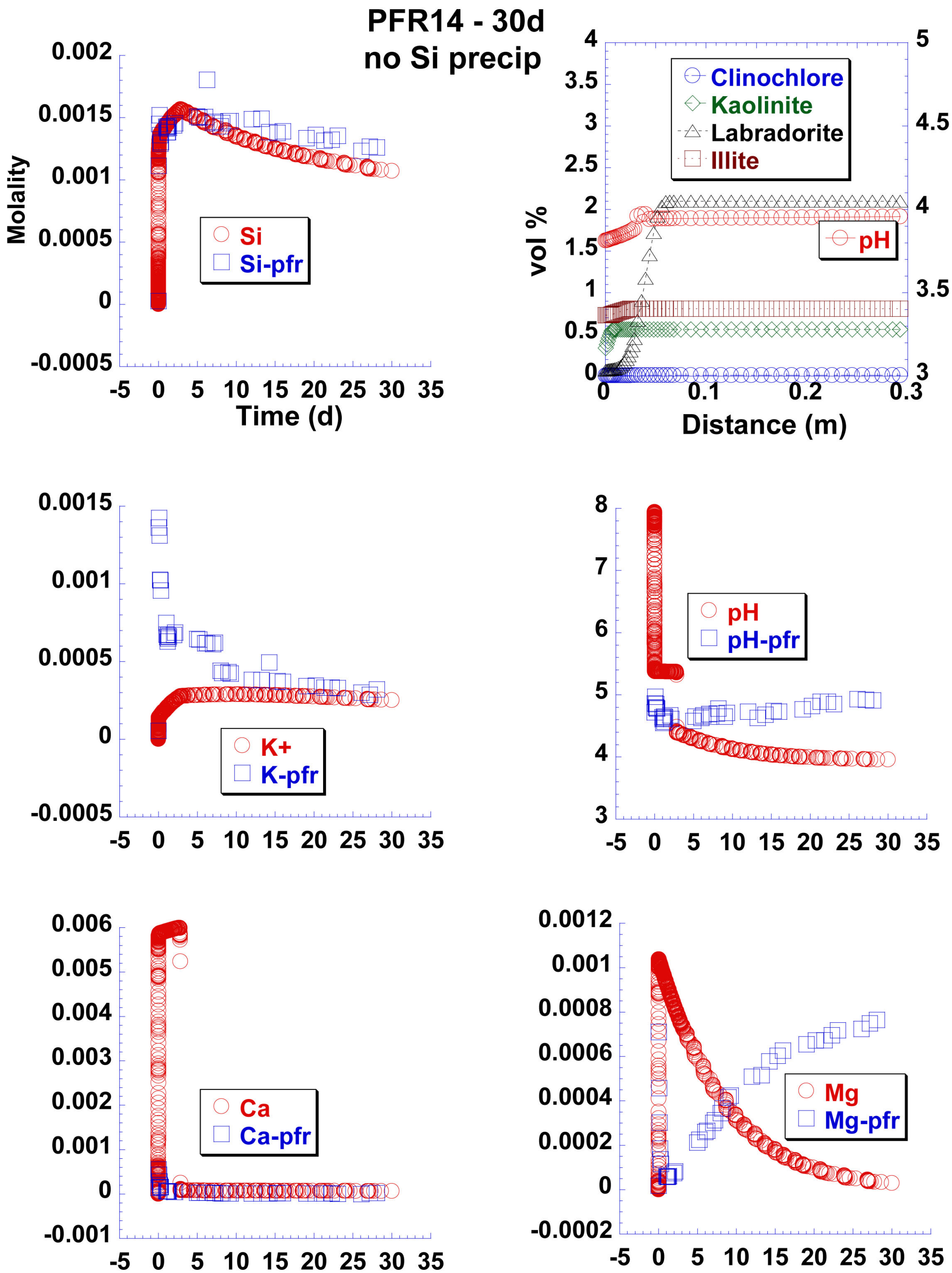


Figure 4. Reactive transport studies. Only non-silica minerals are allowed to grow. With the exception of the upper right graph, simulated results are shown as squares and experimental ones as circles.

What we are most interested in here is the change in solution composition after any early time transient, which may only reflect the temporary conditions that accompany the experiment startup. In **Figure 4,** we see that the K, Ca, and Si values, observed and simulated, track each other following the startup transient, if any. In the case of Si, the prediction and observation are in close agreement throughout the run. In the case of K, the initial transient (pulse in observed K) reflects our initiating the run using distilled water at room temperature (to adjust flow rate and pressure without wasting the NaCl solution—in hindsight, this was being overly conservative). The very short-term pulse could represent initial ion exchange processes in which Na from the brine replaces K in some minerals. The slightly elevated observed K (versus predicted) over the first week suggests that another K-bearing phase may be present (other than K-feldspar and muscovite/illite), or that some fraction of the K-feldspar or illite are present as very fine-grained particles with higher dissolution rate than the bulk mineral. The predicted pulse in Ca (from calcite dissolution) is not seen in the samples, again because we initially used distilled water at room temperature to establish a constant flow rate at run pressure before turning on the furnace. Given that calcite has a retrograde solubility (although dissolution kinetics are prograde), a significant amount of the starting calcite was dissolved before any samples were taken, because we only began sampling when we turned on the furnace. The measured pH is somewhat higher than predicted, in part because the measured pH is at 25°C, while the predicted pH is for150°C. The clear difference between measured and predicted Mg is a direct consequence of the failure of the internal thermocouple (TC) contained in the Ti bomb used to saturate the incoming NaCl solution with high-pressure CO_2. During Day 2 of the run, the TC displayed an open circuit; upon run completion, the disassembled vessel revealed that the TC sheath had split open. The insulator used in the TC is MgO; hence, the measured sample Mg concentration simply reflects the ever-increasing amount of periclase (MgO) that dissolves as the TC sheath continues to split itself open as it hydrates. Fortunately, the system was designed with redundant TCs, and the run continued with full temperature control of the Ti gas equilibration vessel, but with a compromised Mg solution signal in the PFR effluent. The early time differences in effluent composition between prediction and observation can be minimized in future runs by starting right off with the NaCl solution (i.e., no DI water) and by sampling even during the pressure and flow stabilization process. We will follow this new protocol for all subsequent PFR experiments.

We also predict the distribution of several mineral phases in space at the end of the run (see **Figures 3 and 4**) both for cases with and without Si mineral precipitation. If our suggestion that, in fact, no kaolinite grew is correct, then the **Figure 4** (no Si mineral growth) simulation results should match the core samples that will be acquired during the post-mortem of this experiment. The solid phase analyses are still in progress. Note that the code prediction for Ca and Mg solution composition and mineral phases matches the observed effluent composition evolution with time, i.e., the primary mineral sources of Ca (calcite) and Mg (clinochlore) are exhausted prior to the end of the run, resulting in both observed and simulated sample concentrations approaching zero. The accuracy of these assumptions and the correctness of the model itself are precisely what we will test, using the complete set of results from this PFR experiment.

This experiment was successfully completed after running for 30 days. If the solid phase analyses confirm that only mineral dissolution is occurring, then a second experiment at an even higher temperature (to overcome any kinetic inhibition to mineral growth) should provide a good test of kaolinite mineral growth. We will make new reactive transport simulations to design this new experiment next quarter. Note, however, that we can still use the results of this completed experiment to benchmark the code's performance in portraying dissolution and transport, in the absence of mineral growth, at the temperature and pressure conditions of this run.

Work Next Quarter

We will continue investigating the impact of CO_2, as well as other contaminants (such as SO_2, H_2S, NO_2) in the CO_2 waste stream. Our attention will stay focused on work that may help in the design and conduct of the Frio Pilot Project. We plan to complete analysis of the recently completed reactive transport experiment (PFR14) and use the results to begin benchmarking our simulator. To our knowledge, these experiments provide the first really quantifiable tests of any simulator that has been used to date that are directly relevant to CO_2 sequestration. Next quarter, we will also collaborate with TBEG and SandiaTech personnel in making or acquiring cement samples appropriate for durability testing to ensure well bore-seal integrity. See comments on difficulties below.

Task B: Evaluate and Demonstrate Monitoring Technologies

Subtask B-1: Sensitivity Modeling and Optimization of Geophysical Monitoring Technologies

Goals

To (1) demonstrate methodologies for, and carry out an assessment of, the effectiveness of candidate geophysical monitoring techniques; (2) provide and demonstrate a methodology for designing an optimum monitoring system; and (3) provide and demonstrate methodologies for interpreting geophysical and reservoir data to obtain high-resolution reservoir images. The Chevron CO_2 pilot at Lost Hills, California, has been used as an initial test case for developing these methodologies.

Note: This subtask has been completed.

Main Achievements

A methodology for site-specific selection of monitoring technologies was established and demonstrated.

Modeling studies based on well logs from the Liberty Field in south Texas showed that before CO_2 injection, seismic reflection from shale-sand interfaces decreases in amplitude with increasing depth. As CO_2 is injected at shallow depth, reflectivity sharply decreases.

Those numerical studies also indicated that even if a CO_2 wedge were seismically detected because of geometric effects, interpretation of the reflection for fluid properties would be difficult until the horizontal extent of the CO_2 zone exceeds one seismic Fresnel zone.

Results of other modeling work suggested that injection of CO_2 into the Liberty Field (south Texas) formation would produce an easily measurable streaming potential (SP) response.

Subtask B-2: Field Data Acquisition for CO_2 Monitoring Using Geophysical Methods

Goals

To demonstrate (through field testing) the applicability of single-well, crosswell, and surface-to-borehole seismic, crosswell electromagnetic (EM), and electrical-resistance tomography (ERT) methods for subsurface imaging of CO_2.

Previous Main Achievements

- The first test of the joint application of crosswell seismic and crosswell electromagnetic measurements for monitoring injected CO_2 was completed.
- A scoping study of tiltmeter methods to detect and monitor CO_2 injection as part of the Frio Brine Pilot Project (Task E) was refined.
- A time-lapse electrical-resistance tomography (ERT) casing survey was completed in the Vacuum Field, New Mexico, a site where CO_2 injection was taking place.

Accomplishments This Quarter

We tested and deployed a remotely controlled ERT data acquisition system in the field, capable of obtaining full time-lapse datasets on command. The successful deployment will enable frequent surveys for monitoring changes in the field caused by CO_2 injection.

Progress This Quarter

The field deployment in early December 2002 was used to expand the survey area and collect an additional time-lapse dataset. The processing of the data from that deployment is essentially finished. The processed data will act as a baseline for subsequent surveys of the expanded area of coverage.

The remotely controlled ERT data acquisition system, which was previously tested and proved successful, has been redesigned for networking through a satellite data link. The previous link was through a landline and was not suitable for the remoteness of the location at the Hobbs Operating Unit, Buckeye field. The entire system now has been configured in an enclosed trailer that can be parked on site to run unattended. The only external support it will need is standard utility power, which will be available. The satellite dish antenna is mounted on the trailer, so that no surface mount will be needed at the site.

A full test of this system was conducted at LLNL before moving it to the field. The system remained stable and reliable during a full-run test that lasted more than a week. Based on the test results, the trailer-based system was deployed in the field in late April. Datasets were acquired both onsite and remotely over the expanded well pattern, covering the area in which CO_2 injection had recently begun. During and shortly after the deployment, some wells were taken offline. When these wells are re-connected, full time-lapse datasets will be obtained and the results processed and interpreted.

Note: The work this quarter has largely been supported by a separately funded project. Planned work to conclude the CO_2 injection monitoring at the Vacuum Field and the Frio Pilot work scope will need to be revised to reflect the new funding level.

Work Next Quarter

- We will process and analyze time-lapse surveys to monitor changes in the field during CO_2 injection. Interpretation will include comparison to operations and independent reservoir data.
- We will revise plans and design for a tiltmeter survey as part of the Frio Pilot to reflect the new funding level.

<u>Subtask B-3: Application of Natural and Introduced Tracers for Optimizing Value-Added Sequestration Technologies</u>

Goals

To provide methods that utilize the power of natural and introduced tracers to decipher the fate and transport of CO_2 injected into the subsurface. The resulting data will be used to calibrate and validate predictive models utilized for (1) estimating CO_2 residence time, reservoir storage capacity, and storage mechanisms; (2) testing injection scenarios for process optimization; and (3) assessing the potential leakage of CO_2 from the reservoir.

Previous Main Achievements

- Laboratory isotopic-partitioning experiments and mass-balance isotopic-reaction calculations have been done to assess carbon- and oxygen-isotope changes (focused on the influence of sorption) as CO_2 reacts with potential reservoir phases.
- Detailed experiments have been conducted on perfluorocarbon tracer gas-chromatography analytical methods, reproducibility, and sensitivity as a prelude to tracer flow experiments.
- Gas and isotope compositions indicate a slight dilution of injected CO_2 by indigenous reservoir gas in selected wells at the Lost Hills, California site.

Accomplishments This Quarter

- A preliminary mass balance-mixing model of gas and isotope chemistry from the Lost Hills, California. A CO_2 injection test indicated that the contribution of injectate CO_2 to the system can be quantified; increases and decreases in percent CO_2 correlate with periods of CO_2 injection and water flooding, respectively.

Progress This Quarter

We have now completed gas and isotope (carbon and oxygen) analyses of samples obtained from the Chevron Lost Hills CO_2 injection test that took place over a nearly 33-month period (Jan. 2000 to Sept. 2002). To review, gases sampled prior to injection were dominated by CH_4 (~60%) with lesser amounts of CO_2 (~30%) and subordinate amounts of C_2-C_6 (~10%). The $\delta^{13}C$ (PDB) values for CH_4 in pre-injection and all return gases were very similar, ranging from -36 to -42 ‰, with an average of -40.4‰ (± 1.5‰ 1 σ). The initial injection CO_2 had a $\delta^{13}C$ (PDB) value of about -31 ‰ and $\delta^{18}O$ (VSMOW) values of between -1 and -2 ‰. The brine has a $\delta^{18}O$ value of about -1 ‰ VSMOW. The most extensive CO_2 injection was conducted at the end of 2002, with lesser magnitude injections occurring during the end of 2001 and the summer of 2002 (June–August). A major water flood was conducted prior to CO_2 injection (Jan. 2000–Aug. 2000) and also in early 2002.

In previous reports, we have indicated that the gas chemistries plotted on $CO_2 - CH_4 - \Sigma C_2$-C_6 ternaries exhibit a pronounced linear trend, extending from CO_2-rich compositions (nearly 100%) to more CH_4-rich compositions (roughly 60%) indicative of the indigenous reservoir gas. These results are consistent with what one might expect for mixing between reservoir gas and the pure CO_2 injectate gas. The validity of this apparent mixing behavior is further supported if one compares the mole percent CO_2 (normalized to the CO_2-CH_4 binary side line of the ternary) with the carbon isotope compositions of CO_2, as shown in **Figure 5**. This plot shows quite clearly a reasonably well-constrained linear trend between decreasing $\delta^{13}C$ values (dominated by increasing contribution of isotopically light injectate CO_2) with increasing percent CO_2. Within this trend, there are distinct linear groupings unique to a given well. Overall, however, the trend reinforces our hypothesis that gas and isotope chemistries from the Lost Hills injection test are the consequence of binary mixing between injectate and reservoir species.

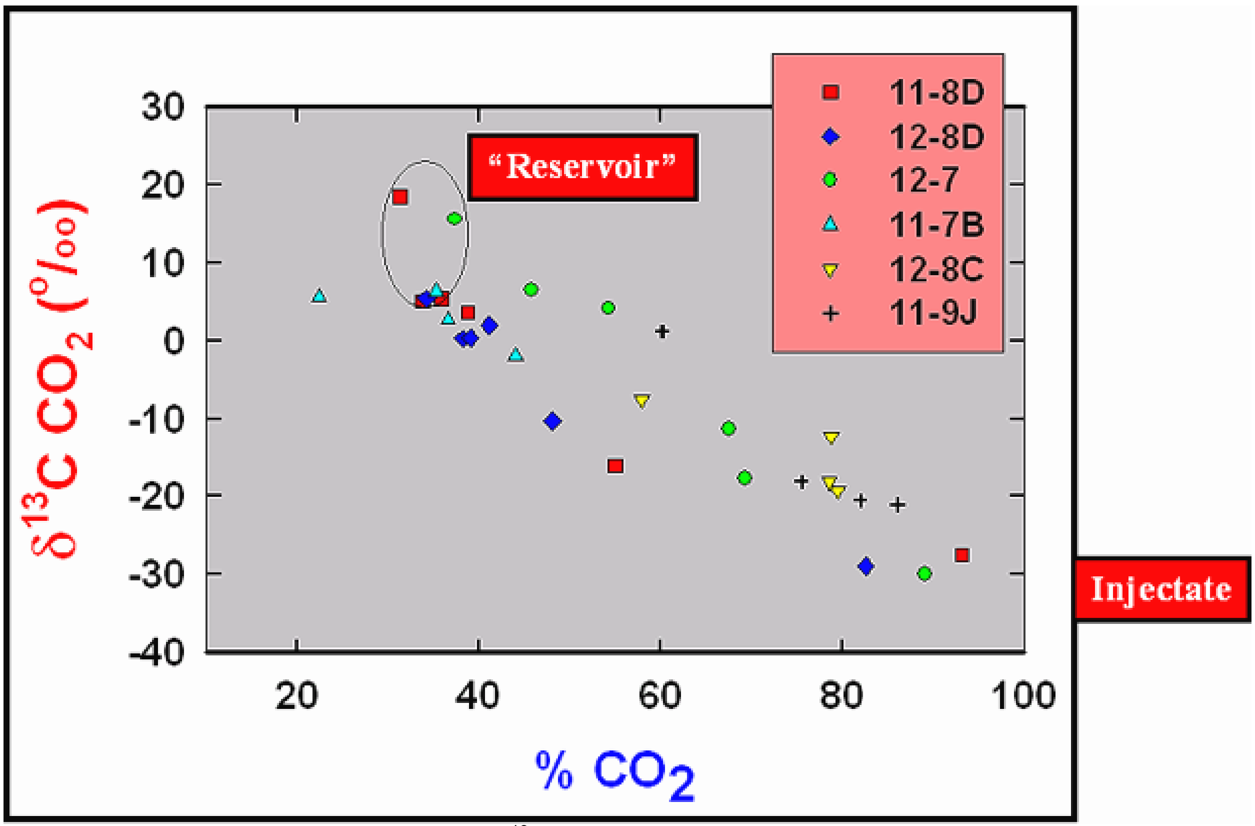


Figure 5. Carbon isotope compositions ($\delta^{13}C$ in per mil) plotted against mole percent CO_2 in the gas samples, corrected to the CO_2-CH_4 binary sideline of the CO_2- CH_4-ΣC_2-C_6 ternary

Assuming this to be the case, mass-balance relationships can be used to quantify the contribution of CO_2 injectate to the system. The mass-balance relationship based only on gas chemistry is given as:

$$X_{CO_2}^{inj} = \frac{Y_{CO_2}^{mix} - Y_{CO_2}^{res}}{(1 - Y_{CO_2}^{res})} \qquad (1)$$

The mass-balance relationship using both isotopes and gas chemistry is given as:

$$X_{CO_2}^{inj} = \frac{(Y_{CO_2}^{mix} \bullet \delta^{13}C_{CO_2}^{mix}) - (Y_{CO_2}^{res} \bullet \delta^{13}C_{CO_2}^{res})}{\delta^{13}C_{CO_2}^{inj} - (Y_{CO_2}^{res} \bullet \delta^{13}C_{CO_2}^{res})} \qquad (2)$$

where X and Y are the mole fractions, and superscripts *inj*, *res*, and *mix* refer to injectate, reservoir, and mixing gas, respectively. If mixing involves only a simple binary system—i.e., injectate with reservoir CO_2—then the values obtained from Equation 1 and 2 should be equal. If not, then some other process may be involved that influences the gas chemistry and/or isotope compositions, such as dissolution and isotopic exchange between gas and water or hydrocarbons. For the most part, estimates from both equations agree fairly well, within ±10%.

The results of the mass balance calculations based on Equation (2) are presented in **Figure 6** in the form of contour maps of the Lost Hills system. The percent contribution of injectate CO_2 to the system is shown for the five sample times: 344–363 days; 683 days; 769 days; 888 days; 1008 days after the initial main water flooding commenced (Jan. 2000). A number of general trends are observed in these plots: (a) the percent contribution of CO_2 is greater for sample times associated with a CO_2 flood; (b) the greatest percent contribution was associated with the largest magnitude CO_2 flood—sample time 333–364 days; (c) Smaller percent contributions of injectate were associated with CO_2 floods of lesser magnitude—683 and 888 days; (d) in general, the percent CO_2 increases from NW to SE in the field; and (e) the contours take on a general strike trend of SW to NE. The geometry and trend in magnitude exhibited by the contours might reflect the fact that high angle faults strike SW–NE through the middle and upper portion of this four 2.5-acre area. These structures could act as flow barriers inhibiting communication between injection wells and production wells located in the middle and northern part of the system; wells to the south clearly have greater communication with the injectors, and thus have higher percent CO_2 values.

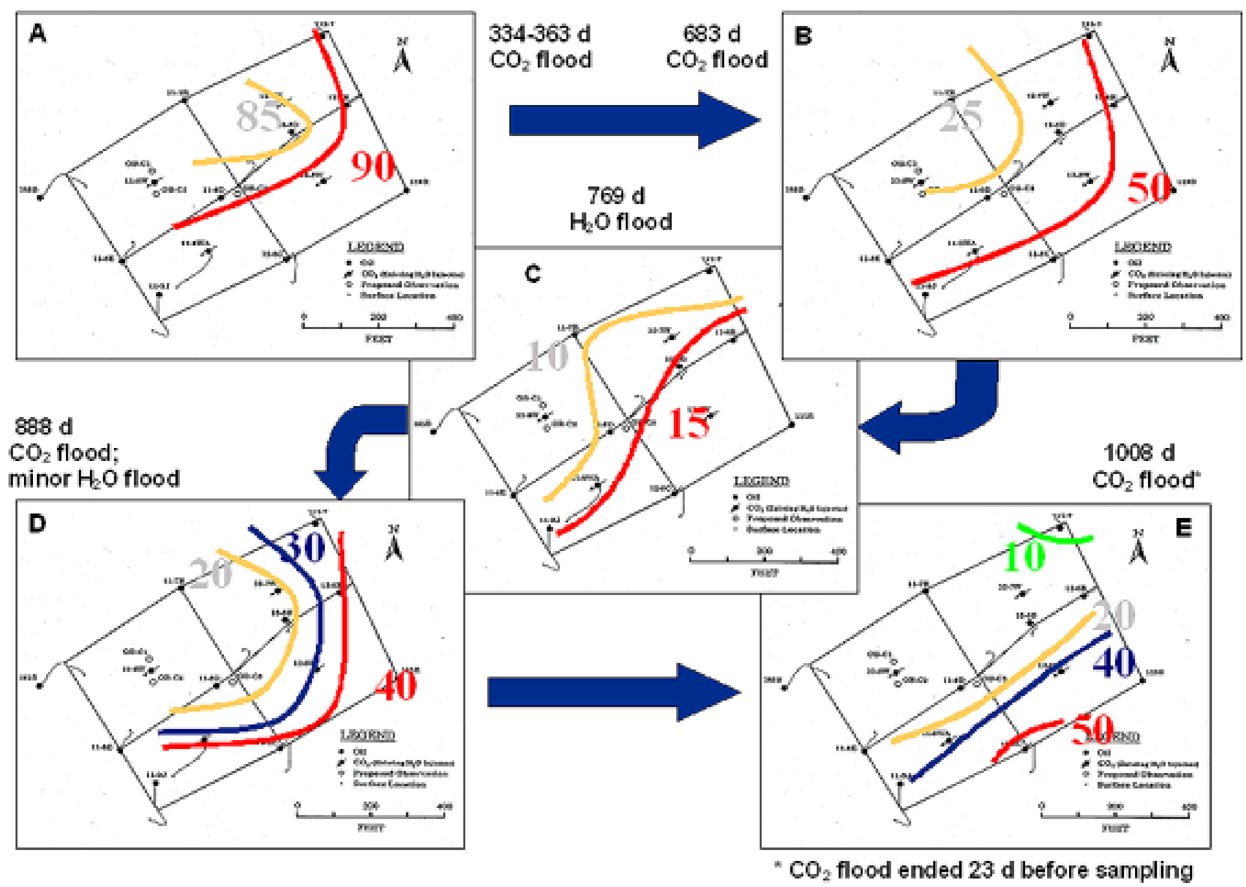


Figure 6. Contour maps showing the percent contribution of CO_2 injectate to the Lost Hills system for five different sample times

Work Next Quarter

- Continue He porosimetry and single PFT tracer flow experiments using Ottawa sand.
- Initiate He porosimetry and single PFT tracer flow experiments using Frio Formation materials.

- Complete analyses of fluid samples; complete modeling of Lost Hills data; submit for publication.
- Continue CO_2 sorption experiments on geological materials.

Subtask B-3A: The Frio Pilot Test Monitoring with Introduced Tracers and Stable Isotopes

Goals

To provide tracer and stable isotope methods that will help quantify the fate and transport of CO_2 injected into the subsurface at the Frio, Texas site (Task E). The resulting data will be used to calibrate and validate predictive models used for (1) estimating CO_2 residence time, reservoir storage capacity, and storage mechanisms; (2) testing injection scenarios for process optimization; and (3) assessing the potential leakage of CO_2 from the reservoir.

Previous Main Achievements

- Gas chemistry and isotope analysis of CO_2 from the BP Hydrogen 1 plant, Texas City, Texas, were conducted in support of permitting documentation needed to inject CO_2 into the Frio formation (Task E).
- Preliminary mineralogical characterization of the Frio Formation sandstone sample was completed

Accomplishments This Quarter

- We prepared the Frio sand for the sequestration flow simulator and loaded the sand into the 20 ft column.
- We developed detailed sampling and experimental plans for both the baseline characterization of the Frio system prior to injection, and for the injection test itself.

Progress This Quarter

At the April Frio CO_2 injection planning meeting in Houston hosted by the Texas Bureau of Economic Geology (TBEG), Oak Ridge National Laboratory (ORNL) provided detailed input on (a) the plan to introduce different suites of PFTs during injection, and (b) the sampling and analytical requirements necessary to observe tracer breakthrough in the monitoring well. A sampling plan was also provided for both fluids and gases that will be collected prior to the injection test to characterize the system, as well as during and after injection has commenced. It was recommended that some on-site chemistry tests (carried out at the Houston Core facility) be performed on the fluids, including (but not limited to) pH, alkalinity, and conductance.

A representative core sample of Frio sandstone (provided by Paul Knox of TBEG) was disaggregated into sand material and loaded into a 20 ft long, 3/8 in internal diameter Monel tube for use in the sequestration flow simulator (SFS). Characterization studies are ongoing to quantify the CO_2 sorption capacity of both the sand and rock chips at high temperature (up to 50^oC) and pressure (a few hundred bars CO_2).

Work Next Quarter

- Continue preparation for the Frio CO_2 injection test.
- Measure the high-temperature, high-pressure CO_2 sorption isotherms on Frio sandstone chips..

Task C: Enhance and Compare Simulations Models

Subtask C-1: Enhancement of Numerical Simulators for Greenhouse Gas Sequestration in Deep, Unmineable Coal Seams

Goals

To improve simulation models for capacity and performance assessment of CO_2 sequestration in deep, unmineable coal seams.

Previous Main Achievements

- Comparisons of the first two sets of simple numerical simulation problems in Part I with pure CO_2 injection and in Part II with flue gas injection have been completed. The participants are CMG's GEM, ARI's COMET3. CSIRO/TNO's SIMEDII, BP's GCOMP, and Imperial College's METSIM2. The results have been posted in the ARC's password-protected Website: http://www.arc.ab.ca/extranet/ecbm/
- Comparisons for the Problem Sets 3 and 4 in Part III (which are more complex problems) have been completed, with participation from CMG's GEM, CSIRO/TNO's SIMED II, ARI's COMET3, GeoQuest's ECLIPSE, BP's GCOMP, and Imperial College's METSIM2.
- Field data obtained from two single-well micropilot tests with pure CO_2 and flue gas injection conducted by the Alberta Research Council (ARC) at the Fenn Big Valley site, Alberta, Canada, have been released to five participants (TNO, BP, CMG, ARI, and Imperial College) for history matching (i.e., Problem Set 5). History matching provides an opportunity to validate new simulation-model developments in a realistic field situation.
- Initial history-matching results from CSIRO/TNO's SIMED II and Imperial College's METSIM2 were collected for the Fenn Big Valley site and were documented.

Accomplishments This Quarter

- Comparison results for Parts I–III from Pennsylvania State University's (Penn State's) PSU-COALCOMP and Shell's MoReS have been collected.
- Field data in Part IV has been released to Penn State for history matching.

Progress This Quarter

Comparison results from Penn State's PSU-COALCOMP for Problem Set 1 in Part I with pure CO_2 injection, Problem Set 2 in Part II with flue gas injection, and Problem Sets 3 and 4 in Part III with more complex problems have been collected. Also, comparison results have been collected from Shell's MoReS for the first two sets of simple numerical simulation problems in Part I with pure CO_2 injection and in Part II with flue gas injection. These results are being documented and will be updated in the Alberta Research Council's (ARC's) password-protected website: http://www.arc.ab.ca/extranet/ecbm/.

Field data obtained by ARC at the Fenn Big Valley site, Alberta, Canada for a single-well micropilot test with pure CO_2 injection has been released to Penn State under a confidential agreement to use the data for the purpose of model comparison only.

History matching of the ARC's field data continues, using GEM with a new algorithm developed by ARC to describe the permeability variation of coal during CO_2 and flue gas injection.

Work Next Quarter

ARC will continue to collect and document field history-matching results from participants who have access to the field data.

Subtask C-2: Intercomparison of Reservoir Simulation Models for Oil, Gas, and Brine Formulations

Goals

To stimulate the development of models for predicting, optimizing, and verifying CO_2 sequestration in oil, gas, and brine formations. The approach involves: (1) developing a set of benchmark problems; (2) soliciting and obtaining solutions for these problems; (3) holding workshops that involve industrial, academic, and laboratory researchers; and (4) publishing results.

Note: This subtask has been completed.

Main Achievements

- A workshop on the code intercomparison project was held at Berkeley Lab on October 29–30, 2001, with the initial modeling results by different groups showing reasonable agreement for most problems.
- The final report on the code intercomparison study was issued.
- A detailed report with Berkeley Lab results on the saline aquifer test problems was completed.

Task D: Improve the Methodology and Information for Capacity Assessment

Goals

To improve the methodology and information available for assessing the capacity of oil, gas, brine, and unmineable coal formations; and to provide realistic and quantitative data for construction of computer simulations that will provide more reliable sequestration-capacity estimates.

Previous Main Achievements

- A new definition of formation capacity, incorporating intrinsic rock capacity, geometric capacity, formation heterogeneity, and rock porosity, was developed for use in assessing sequestration capacity.
- Many modeling studies of the Frio Brine Pilot Experiment (Task E) were completed, assuming different CO_2 injection scenarios and geologic models.
- We developed a basin-scale conceptual model of geologic complexity for the Frio Brine Pilot Experiment site (Task E). Quantitative data has been compiled to probabilistically and deterministically create a simulation for the basin.
- We extended the modeling studies of the post-injection period for the Frio Brine Pilot Experiment from one year to 100 years. As in previous studies, the choice of characteristic curves has a strong impact on CO_2 plume evolution

Accomplishments This Quarter

- Grid effects on numerical simulation of CO_2 injection and storage were investigated.
- Well-test scenarios for site-characterization prior to Frio brine pilot were simulated

Progress This Quarter

Grid Effects. To assess the accuracy of numerical model results, three grid-effect studies were conducted, examining:

- Vertical grid resolution
- Lateral grid resolution
- Grid orientation

For the vertical grid resolution study, the Umbrella Point model (described in previous reports) was used. The model is composed of ten depositional layers, which interleave mostly sand layers and mostly shale layers, providing potential pathways for preferential flow of buoyant CO_2. The model simulates CO_2 injection at a rate of 680,000 metric tons per year (21.6 kg/s) for a period of 20 years.

Figure 7 shows a time sequence of spatial distributions of CO_2 in the immiscible gas-like phase during the injection period for the basic model, in which there is one grid layer for each depositional layer. Strongly preferential flow occurs, as buoyant CO_2 finds gaps in the shale layers and moves upward from the injection interval in the lower half of the model. **Figure 8** shows the analogous time sequence for a model with a finer vertical grid, with three grid layers for each depositional layer. The overall patterns of plume development are similar for the coarse and fine grids, but the fine-grid model shows higher concentrations of CO_2 because it allows resolution of buoyancy flow within individual sand channels.

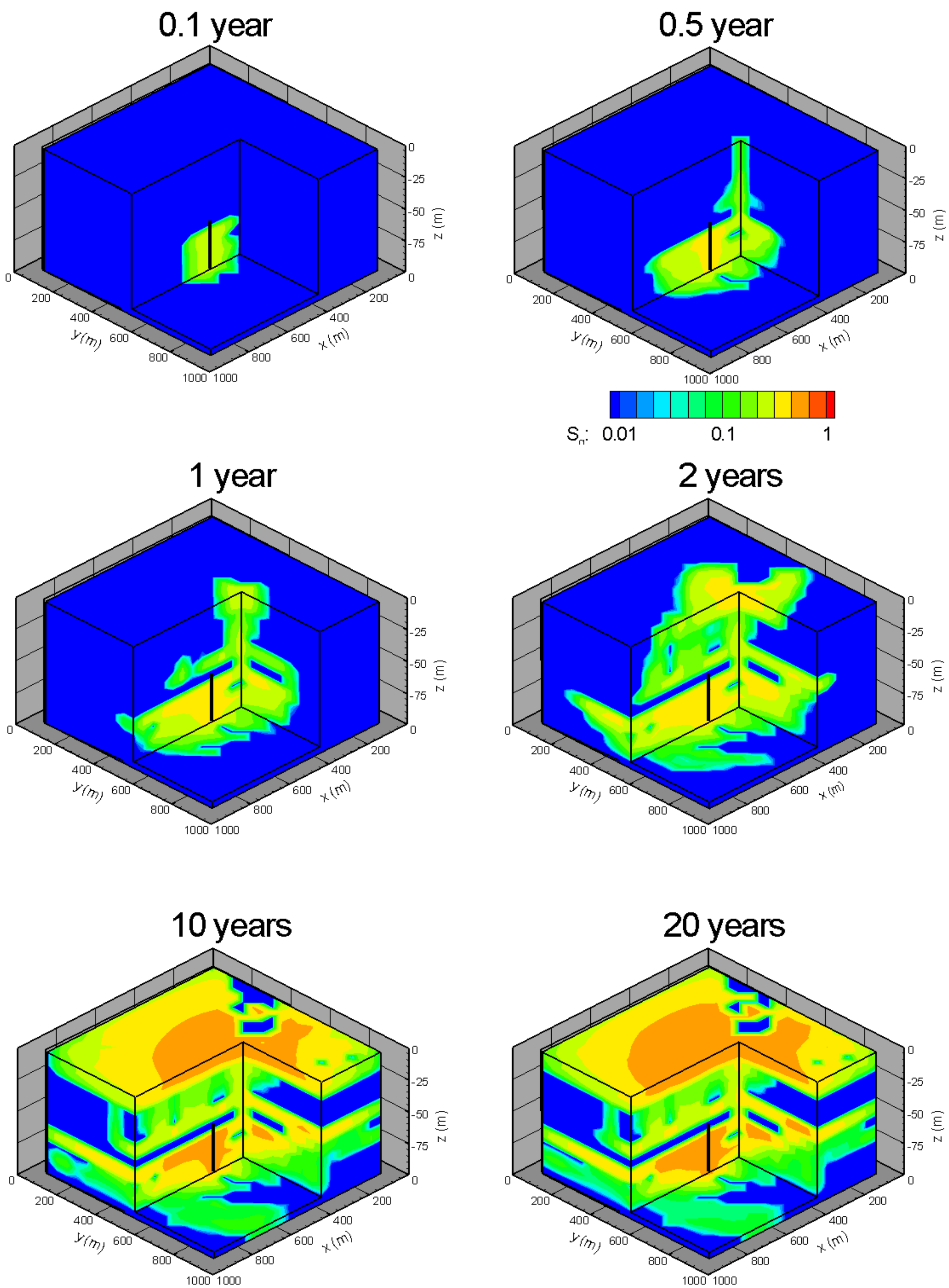


Figure 7. Spatial distributions of gas-phase CO_2 obtained from the basic Umbrella Point model with one grid layer per depositional layer

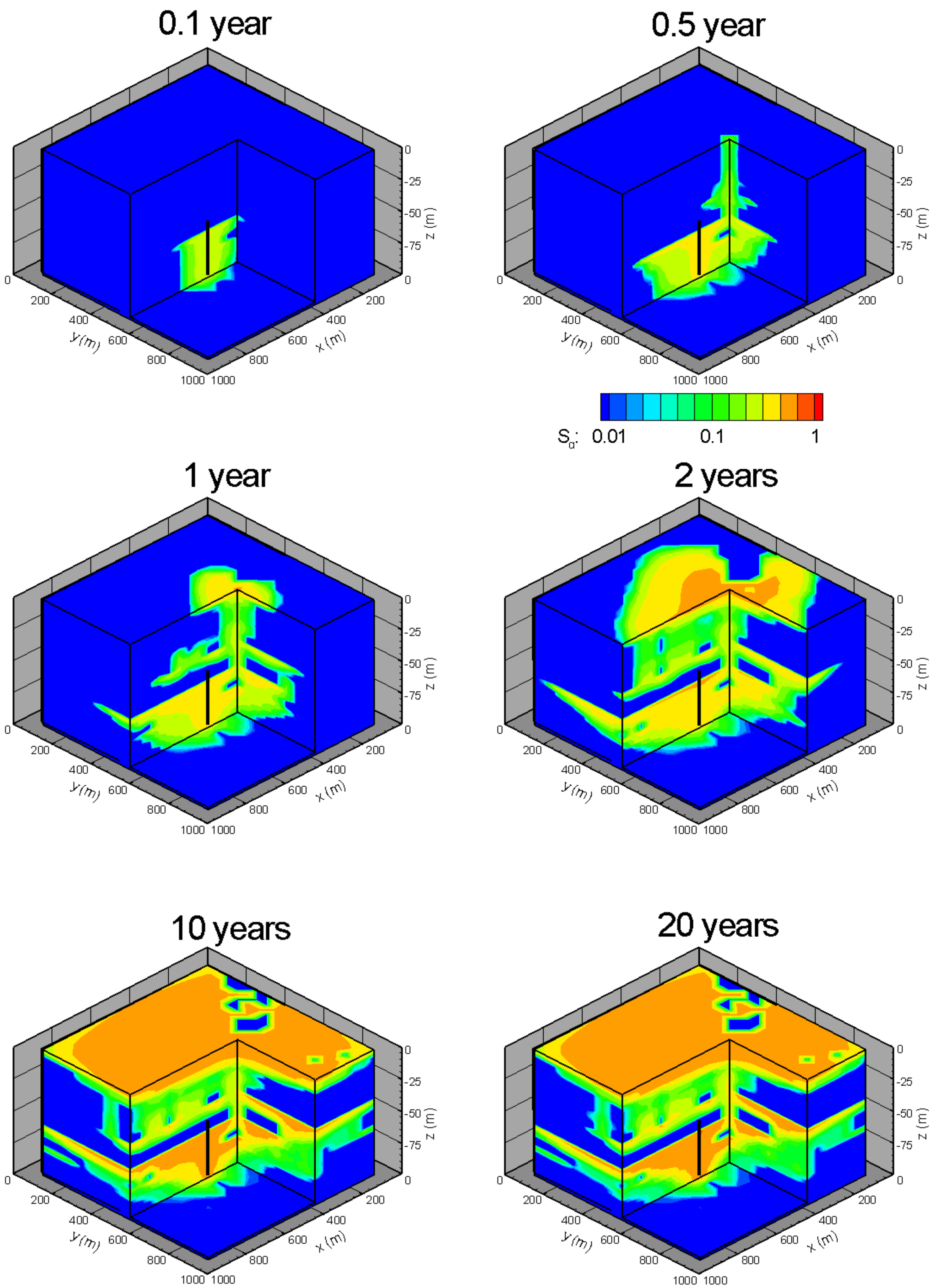

0.1 year
0.5 year
1 year
2 years
10 years
20 years
y (m)
x (m)
z (m)
0
-25
-50
-75
200
400
600
800
1000
S_a: 0.01 0.1 1

Figure 8. Spatial distributions of gas-phase CO_2 obtained from the finer Umbrella Point model with three grid layers per depositional layer

Comparison of **Figures 7 and 8** shows that after one year, the fine-grid model appears to contain more CO_2. To quantify CO_2 sequestration, we use the capacity factor *C*, defined as the fraction of a specified volume of the subsurface containing CO_2. Capacity factor can be broken down by phase: $C = C_g + C_l$, where C_g is the fraction of the subsurface containing CO_2 in the gas-like phase and C_l is the fraction containing CO_2 dissolved in the aqueous phase. We have

$$C_g = \langle S_g \phi \rangle \tag{3}$$

$$C_l = \langle S_l X_l^{CO2} \rho_l / \rho_g \phi \rangle \tag{4}$$

where S_g and S_l are gas and liquid saturations, respectively; ϕ is porosity, X_l^{CO2} is the mass fraction of CO_2 dissolved in the aqueous phase; ρ_l and ρ_g are liquid- and gas-phase densities, respectively; and the angle brackets indicate an average over the specified volume. For the Umbrella Point model, the averaging volume is simply the model volume.

The capacity factor versus time for the basic and fine-grid models is shown in **Figure 9**. Note that *C* increases linearly until the first CO_2 reaches the outer boundary of the model (the spill point) at about two years. Somewhat later, a quasi-steady state is reached in which the injection rate at the well nearly balances CO_2 flow out the lateral model boundaries. The figure indicates that the amount of CO_2 dissolved in the aqueous phase is not very sensitive to the grid resolution, but significantly more gas-like CO_2 remains in the fine-grid model where intra-sand channel buoyancy flow can be resolved.

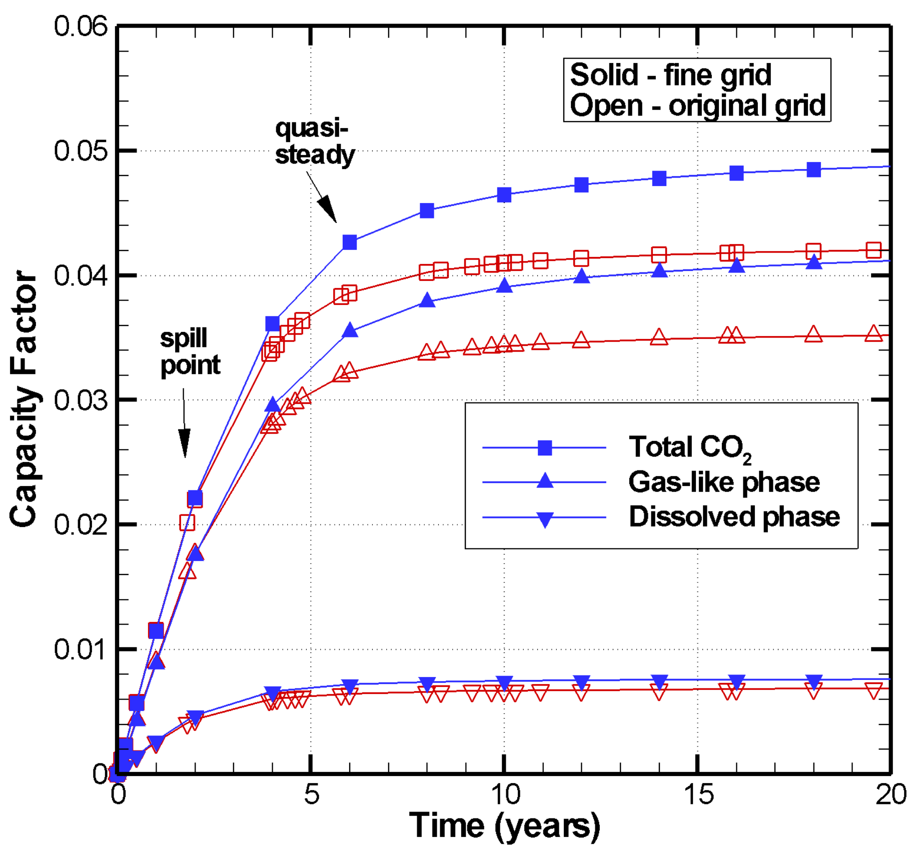


Figure 9. Capacity factor (fraction of subsurface containing CO2) as a function of time during a 20-year injection period, for the original (coarse) and fine Umbrella Point models.

The lateral-grid-resolution and grid-orientation studies use the South Liberty model, developed to study the upcoming Frio brine pilot. **Figure 10** shows gas-phase CO_2 plume development for the basic South Liberty model with a sequence of plan views of the top of the upward-coarsening sand, which is the top of the injection interval. During the 20-day injection period, the distribution of CO_2 is nearly symmetric around the injection well. However, after injection ends, the buoyant flow of CO_2 updip becomes obvious. After one year, the bulk of the plume has moved updip of both the injection and monitoring wells. The irregular shape at the leading edge of the plume reflects flow around a shaley region.

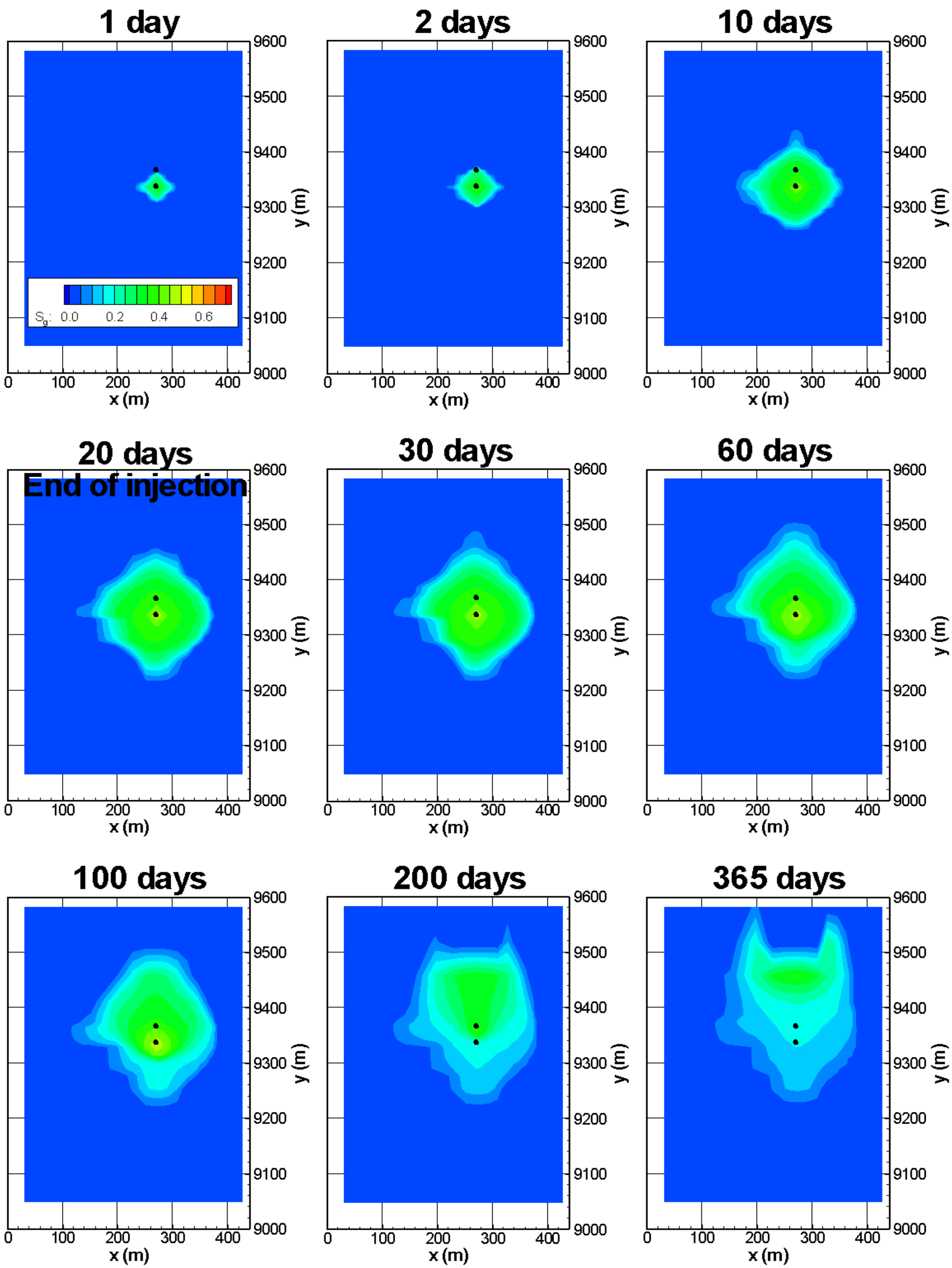


Figure 10. Time sequence of gas-phase CO_2 distributions at the top of upward-coarsening sand in the South Liberty model, with five-point differencing, a non-uniform grid, and generic characteristic curves. Positive y-direction is updip; injection and monitoring wells are shown.

During the injection period, the plan view of the CO_2 plume actually looks more diamond-shaped than circular (**Figure 10**, top row). The model has homogeneous properties close to the injection well, so the lack of radial symmetry may result from grid effects. To investigate the role of the grid, we developed two alternative models.

The diamond-shape of the early CO_2 plume is typical of the preferential flow that arises along the axis directions in a rectangular grid that uses five-point differencing for lateral connections (i.e., four lateral connections for each gridblock, one to each of its nearest neighbors). Using nine-point differencing for lateral connections (i.e., eight lateral connections for each grid block, the usual four nearest neighbors, plus the four nearest diagonal neighbors) can ameliorate this problem.

The implementation of nine-point differencing requires a laterally regular grid with square gridblocks. In the original grid, lateral spacing ranges from 2 m at the wells, to about 60 m near the closed edges of the model, to several hundred meters to the southwest, where the model extends far enough to act unbounded. A new grid with a uniform lateral spacing of 7.5 m was created. It has a constant-pressure boundary rather than extending far in the down-dip direction—a concession to the size limitations of the computer being used for the simulations. Note, however, that the new grid will not resolve near-well behavior as well as the original one.

Figures 11 and 12 show plume development for the uniform grid with five-point and nine-point differencing for lateral connections, respectively. During the injection period, nine-point differencing produces a more circular plume, as expected. An unanticipated result is that during the post-injection period, the added lateral flow enabled by nine-point differencing slightly increases updip translation of the plume.

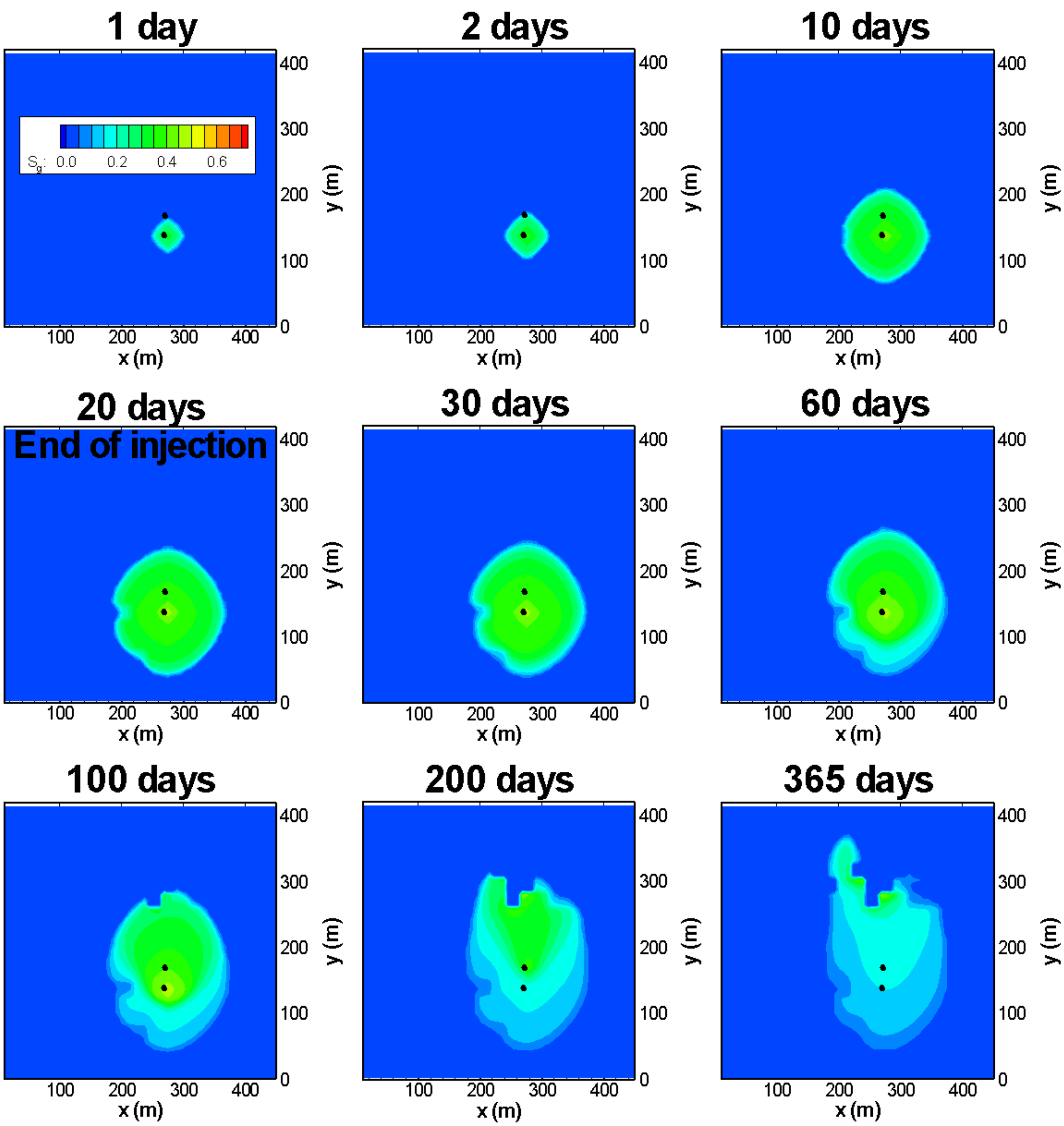


Figure 11. Time sequence of gas-phase CO_2 distributions at the top of upward-coarsening sand in the South Liberty model, with five-point differencing, a uniform grid, and generic characteristic curves. Positive y-direction is updip; injection and monitoring wells are shown.

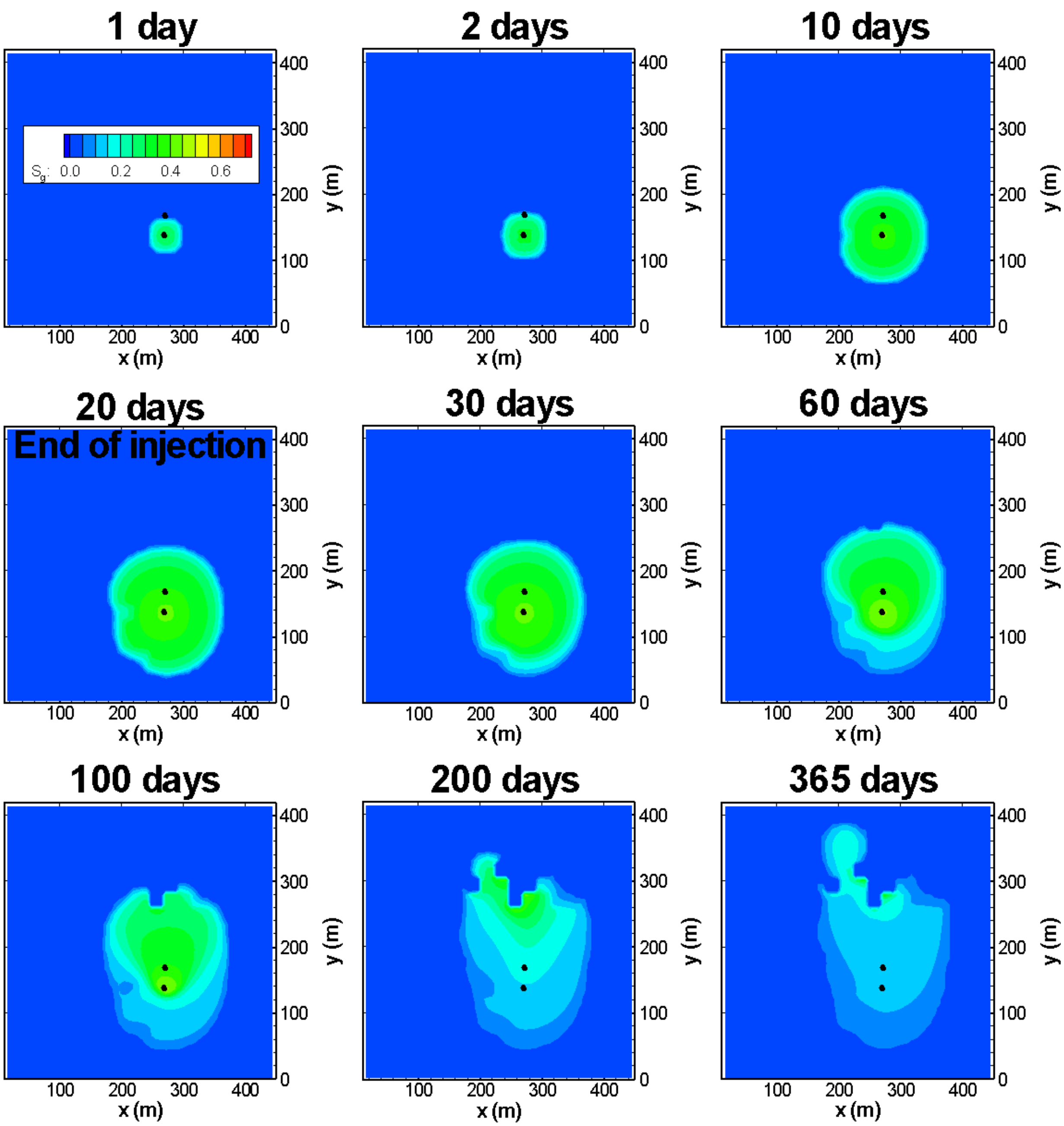


Figure 12. Time sequence of gas-phase CO_2 distributions at the top of the upward-coarsening sand in the South Liberty model, with nine-point differencing, a uniform grid, and generic characteristic curves. Positive y-direction is updip; injection and monitoring wells are shown.

Comparison to the plume resulting from the non-uniform grid (**Figure 10**) makes it apparent that the preferential flow in the grid axis directions is exacerbated by the coarsening of the grid away from the wells, which further distorts the shape of the plume by enhancing spreading (due to numerical dispersion). Spreading caused by phase dispersion is an important aspect of plume evolution; it is undesirable to mask this process with spurious numerical effects. Moreover, with the more accurate plume depiction afforded by a finer grid, subtle irregularities in the plume shape may be attributed to geological features. In particular, the small indentations in the lower left quadrant of the plume, visible starting at 20 days, reflect gaps in the overlying thin shale layer, where CO_2 is leaking into the upper half of the model.

Well test simulations. Pumping and injection tests accompanied by pressure-transient monitoring will be essential in site characterization for the upcoming brine pilot test (CO_2 injection in a brine-bearing sand of the fluviodeltaic Frio formation). Site characterization goals include:

- Estimation of single-phase flow properties
- Determination of appropriate lateral boundary conditions for the subvertical faults bounding the pilot site
- Assessment of the integrity of inter-sand shale layers
- Analysis of ambient-phase conditions within the formation (although nominally brine-saturated, the pilot-site sands may harbor immobile gas-phase or dissolved hydrocarbons).

The Dec. 02–Feb. 03 report outlined the sequence of well tests proposed to occur prior to CO_2 injection. The short-term (less than one day) well tests are designed to improve our understanding of the *in situ* composition and phase conditions for the nominally brine-saturated sands of the upper Frio. They can be simulated with radial models. Figure 13 shows an example, comparing pressure responses at the pumping and monitoring wells for a pumping rate of 3.15 kg/s (50 gpm), for models with no gas, dissolved gas, 5% gas-phase saturation, and 10% gas-phase saturation (the residual gas saturation, S_{gr}, is 23%, so the gas is immobile). The addition of an immobile gas phase slows the pressure response at both wells by virtue of the increased compressibility of a two-phase system. When the pressure decrease at the pumping well becomes large enough, dissolved gas begins to exsolve, increasing gas saturation. When gas saturation exceeds S_{gr}, the gas phase becomes mobile. This phenomenon has two effects: first, the gas can be pumped out of the formation, so the saturation stabilizes at a value just above S_{gr}. Second, the mobile gas phase interferes with the liquid phase, decreasing its relative permeability and correspondingly increasing the pressure change. At the monitoring well, the pressure decrease caused by pumping is too small to cause exsolution, so gas saturations remain constant.

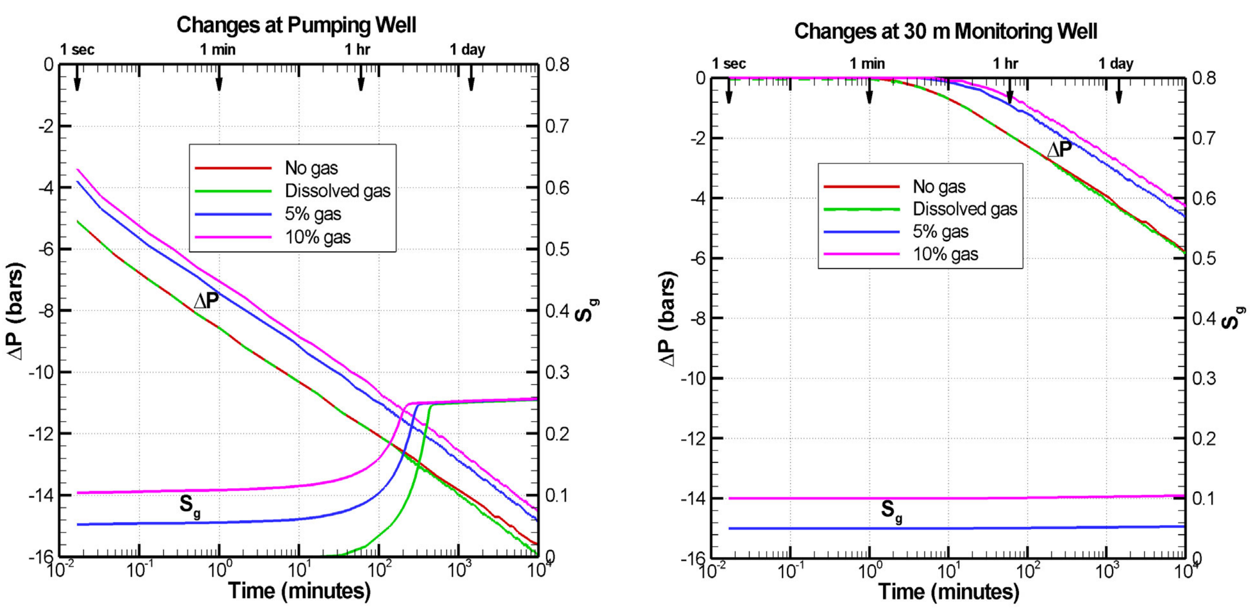


Figure 13. Simulated well-test response for a constant-rate pumping test, for different *in situ* phase conditions.

Simulation results for an injection test for the same four cases are shown in **Figure 14**. As before, the pressure response is slower when a gas phase is present. As pressure increases due to injection, gas around the injection well dissolves. The transition to a liquid-phase system is reflected by a small jump in the pressure transients. Gas saturation at the monitoring well remains constant.

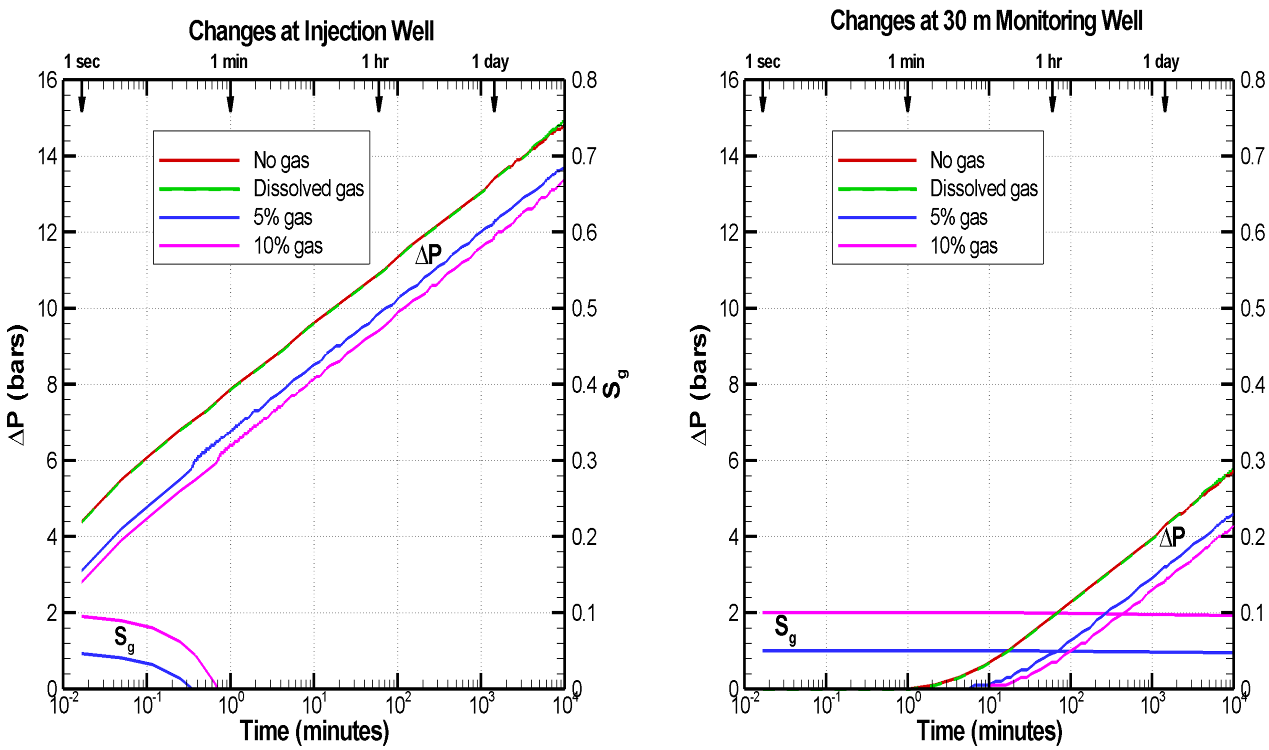


Figure 14. Simulated well-test response for a constant-rate injection test, for different *in situ* phase conditions

Work Next Quarter

Further modeling studies will continue on two fronts:

- Capacity investigations using generic models that are designed to capture essential features of formations suitable for sequestration
- Simulations of the planned Frio brine pilot to be conducted at the South Liberty field, incorporating more detailed test specifications, as they are developed.

Task E: Frio Brine Pilot Project

Goals

To perform numerical simulations and conduct field experiments at the Frio Brine Pilot site, near Houston, Texas, that:

- Demonstrate that CO_2 can be injected into a saline formation without adverse health, safety, or environmental effects.
- Determine the subsurface location and distribution of the cloud of injected CO_2.
- Demonstrate understanding of conceptual models.
- Develop the experience necessary for the success of large-scale CO_2 injection experiments.

Note: This task does not include work being done by TBEG for the project "Optimal Geological Environments for Carbon Dioxide Disposal in Brine Formations (Saline Aquifers) in the United States," funded under a separate contract.

Previous Main Achievements

- An initial planning workshop was held at BEG (Austin, Texas) on July 8–9, 2002, to explore the interrelationships among the modeling and monitoring techniques proposed by the GEO-SEQ team for conducting the Frio Brine Pilot experiment. A time line and a more detailed plan for implementation of modeling and monitoring techniques were developed.
- Permit preparation for the project has been completed, with substantive input from the GEO-SEQ team.

Accomplishments This Quarter

- The Frio Brine Pilot project team met on April 23–24 in Houston, Texas, to update and add details to the drilling, sampling, logging, monitoring, and data interpretation activities planned for the Fall 2003 CO_2 injection test.
- More detailed plans have been created to integrate the various GEO-SEQ experiments with the well design and test schedule.

Progress This Quarter

The Task E team met on April 23–24 in Houston and at the field site to revise the well testing plan. The team was joined by Schlumberger Research staff Austin Boyd and T.S. Ramakrishnan to provide information about downhole technologies; NETL staff Art Wells, Grant Bromhall, and Rod Diehl, who will participate in monitoring and observation activities during the experiment; and Sandia Technologies staff Donald Stehli, Dan Collins, and Philip Papadeas who are coordinating the well design and field activities.

Work Next Quarter

The report to support the Class 5 permit application to Texas Commission on Environmental Quality will be completed next quarter. We will continue work with stakeholders in the Houston area. We plan to enter and assess the condition of the Number 4 well, which is the proposed monitoring well.